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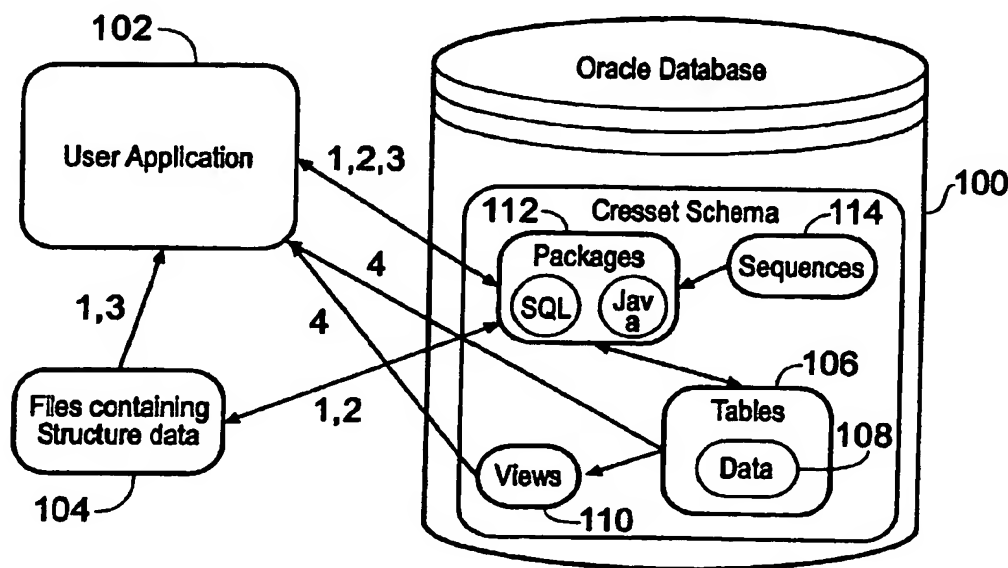
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(54) Title: SEARCHABLE MOLECULAR DATABASE



(57) Abstract: A computer system comprising a database (100) having a plurality of records is provided. Each record comprises a filed point representation representing field extrema for a conformation of a chemical structure. The database may include records for multiple conformations of the same chemical structure. Each record can have a searchable index of the filed point representation. In one embodiment the index is bit string. An indexing mechanism for generating an index, a searching mechanism for searching the database and a graphical user interface to enable a user to interface with the database (100) are also provided.



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ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO,
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A. CLASSIFICATION OF SUBJECT MATTER

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B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

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EPO-Internal, WPI Data, PAJ, INSPEC, COMPENDEX

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X Y	<p>GB 2 317 030 A (XENOVA LTD) 11 March 1998 (1998-03-11)</p> <p>page 4, line 9 - line 11 page 7, line 24 - line 29 page 8, line 35 - page 9, line 15 page 11, line 6 - line 11 --- -/--</p>	<p>1-7, 20, 24-31 8-19, 21-23, 32-43</p>



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Patent family members are listed in annex.

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Y	<p>XUE L GODDEN J W BAJORATH J: "Database searching for compounds with similar biological activity using short binary bit string representation of molecules" JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES, AMERICAN CHEMICAL SOCIETY, COLOMBUS, OHIO, US, vol. 39, no. 5, 1999, pages 881-886, XP002958748 ISSN: 0095-2338 abstract page 881, left-hand column, line 17 -right-hand column, line 5 page 882, left-hand column, line 1 - line 12</p>	<p>8-19, 21-23, 32-43</p>
A	<p>FLOWER D R: "On the properties of bit string-based measures of chemical similarity" JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES, MAY-JUNE 1998, ACS, USA, vol. 38, no. 3, pages 379-386, XP002267834 ISSN: 0095-2338 page 380, section "Encoding Structural Information in Bit Strings"</p>	<p>1,8,12, 16,17, 32,33, 39,40</p>
A	<p>"XEDs : eXtended Electron Distribution" CRESSET BIOMOLECULAR DISCOVERY LTD. WEB SITE, 'Online! 5 June 2002 (2002-06-05), XP002267833 Retrieved from the Internet: <URL:http://web.archive.org/web/20020605204228/cresset-bmd.com/Science1.html> 'retrieved on 2004-01-21! page 1, paragraph 1 page 2, section "Validation" to page 3, line 2</p>	<p>1-43</p>

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